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Study of Water Cluster-Amorphous Silica Collisions in the Extreme Space Environment Using the ReaxFF Reactive Force Field Molecular Dynamics Simulation Method

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Abstract : The concept of high velocity particle impact on the spacecraft surface materials has been one of the important issues in the design of such materials. Among these particles, water clusters might be the most abundant and the most important particles to be studied. The importance of water clusters is that upon impact on the surface of the materials, they can cause damage to the material and also if they are sub-cooled water clusters, they can attach to the surface of the materials and cause ice accumulation on the surface which is very problematic in spacecraft and also aircraft operations. The dynamics of the collisions between amorphous silica structures and water clusters with impact velocities of 1 km/s to 10 km/s are studied using the ReaxFF reactive molecular dynamics simulation method. The initial water clusters include 150 water molecules and the water clusters are collided on the surface of amorphous fully oxidized and suboxide silica structures. These simulations show that the most abundant molecules observed on the silica surfaces, other than reflecting water molecules, are H3O+ and OH- for the water cluster impacts on suboxide and fully oxidized silica structures, respectively. The effect of impact velocity on the change of silica mass is studied. At high impact velocities the water molecules attach to the silica surface through a chemisorption process meaning that water molecule dissociates through the interaction with silica surface. However, at low impact velocities, physisorbed water molecules are also observed, which means water molecule attaches and accumulates on the silica surface. The amount of physisorbed waters molecules at low velocities is higher on the suboxide silica surfaces. The evolution of the temperatures of the water clusters during the collisions indicates that the possibility of electron excitement at impact velocities less than 10 km/s is minimal and ReaxFF reactive molecular dynamics simulation can predict the chemistry of these hypervelocity impacts. However, at impact velocities close to 10 km/s the average temperature of the impacting water clusters increase to about 2000K, with individual molecules oocasionally reaching temperatures of over 8000K and thus will be prudent to consider the concept of electron excitation at these higher impact velocities which goes beyond the current ReaxFF ability.

Keywords : spacecraft materials, hypervelocity impact, reactive molecular dynamics simulation, amorphous silica
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